Modeling dynamics of organic carbon and nitrogen removal during aeration interruption in aerated horizontal flow treatment wetlands – Supplementary Information

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1 Experiments

1.1 Site and Pilot–scale Systems

Figure 1: Schematic of the experimental site, systems and corresponding modeling scenarios. Modified from Nivala et al. (2013). with Permission from Elsevier.
Figure 2: Schematic of the experimental systems (width of 1.2 m) used at the site and corresponding model domains. Modified from Boog et al. (2019); With permission from Elsevier.
1.2 Hydraulic Flow Data

Figure 3: Hydraulic in- and outflow rates of the wetland HA during May 2015 to February 2016. The deviating values from September 28th to October 15th 2015 were related to a site malfunction. These data were excluded from further analysis. Corresponding median hydraulic inflow and outflow rates were 0.578 m$^{-3}$ d$^{-1}$ and 0.576 m$^{-3}$ d$^{-1}$.

1.3 Water Quality Data

2 Process Model

2.1 Imputation of TOC for Influent and Effluent Samples

TOC was not measured consistently during the aeration experiment in June to August 2015, therefore, TOC was imputed for the influent and effluent samples of the wetland HA. The imputation was based on ratios of TOC to DOC computed from measurements of routine monitoring during June to August 2015. Mean TOC/DOC for influent and effluent of HA were 1.4 and 1.5, respectively.

2.2 Imputation of COD$_t$ and COD$_s$

The biokinetic reactions of the process model are based on chemical oxygen demand (COD). As COD$_t$ and COD$_s$ were not measured consistently, measured TOC and DOC values were converted to total COD (COD$_t$) and soluble COD (COD$_s$), respectively. Influent and effluent COD$_t$ were imputed by regression models that were calibrated using measurements for COD$_t$, TOC, DOC, CBOD$_5$ of the routine monitoring during January to December 2015; corresponding COD$_s$ were imputed by combining ratios of measured TOC/DOC.
Figure 4: Preprocessed (outliers excluded, imputations for CODₜ, CODₜₛ, BCOD, TOC) influent wastewater quality during May 2015 to February 2016. All values in mg/L, except T_field (°C). NO₃–N and NO₂–N were always less than or equal to 0.25 mg/L.
and COD_t/COD_s obtained by Boog et al. (2019). COD_t, COD_s of pore water samples were imputed using ratios COD_t/TOC and COD_s/DOC obtained by Boog et al. (2019).

### 2.2.1 Imputation of COD_t of Influent and Effluent Samples

Regression equations for the influent and effluent of HA as well as for the effluent of HMc were obtained to impute COD_t when it was not measured.

**Figure 5:** Imputed and measured COD_t data for wetland HA (HA-OUT), HMc (HMc-OUT) and influent (SEP-OUT). Data and regression models based on Boog et al. (2019). Mod1 and mod2 represent the concentration of COD_t computed using the regression models defined in the subsequent sections.

### 2.2.1.1 Regression Models for SEP-OUT

**SEP-OUT mod1**

```r
## Family: gaussian
## Link function: identity
##
## Formula:
## COD ~ T_field + CBOD5 + TOC + s(year_day, fx = TRUE, bs = "cr", k = 6)
##
## Parametric coefficients:
## Estimate Std. Error t value Pr(>|t|)
```

---

5
## (Intercept) -3.6102 87.2188 -0.041 0.967
## T_field 7.3924 6.3419 1.166 0.255
## CBOD5 0.2022 0.1671 1.210 0.238
## TOC 2.3041 0.3222 7.151 1.71e-07 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
##
## Approximate significance of smooth terms:
## edf Ref.df  F  p-value
## s(year_day) 5 5 8.38 5.04e-05 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
##
## R-sq.(adj) = 0.934  Deviance explained = 95%
## GCV = 1074.5  Scale est. = 578.9  n = 34

SEP-OUT mod2
##
## Family: gaussian
## Link function: identity
##
## Formula:
## COD ~ T_field + TOC + s(year_day, fx = TRUE, bs = "cr", k = 6)
##
## Parametric coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) -3.0626 83.7600 -0.037 0.971
## T_field 7.8875 6.1562 1.281 0.211
## TOC 2.6573 0.1471 18.069 <2e-16 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
##
## Approximate significance of smooth terms:
## edf Ref.df  F  p-value
## s(year_day) 5 5 17.15 1.22e-07 ***
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 '' 1
##
## R-sq.(adj) = 0.934  Deviance explained = 94.8%
## GCV = 945.14  Scale est. = 566.52  n = 35

2.2.1.2 Regression Models for HA-OUT

HA-OUT mod1
##
## Family: gaussian
## Link function: identity
##
## Formula:
## COD ~ T_field + CBOD5 + TOC
##
## Parametric coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 5.7327270 7.1194142 0.805 0.428

6
## Regression Models for HMc-OUT

### HMc-OUT mod1

```r
## Family: gaussian
## Link function: identity

## Formula:
## COD ~ T_field + CBOD5 + TOC + DOC

## Parametric coefficients:
## Estimate Std. Error t value Pr(>|t|)
## (Intercept) 14.20919 4.51896 3.144 0.00402 **
## T_field -0.12305 0.09119 -1.349 0.18845
## CBOD5 -0.5165 0.65714 -0.839 0.40858
## TOC 1.11767 0.66376 1.684 0.10374

## R-sq.(adj) = 0.402 Deviance explained = 47.9%
## GCV = 7.7811 Scale est. = 5.6287 n = 32
```
## Family: gaussian
## Link function: identity

## Formula:
COD ~ T_field + TOC + s(year_day, fx = TRUE, bs = "cr", k = 6)

## Parametric coefficients:

| Estimate | Std. Error | t value | Pr(>|t|) |
|----------|------------|---------|----------|
| (Intercept) | 16.1311 | 6.0271 | 2.676 | 0.0129 * |
| T_field | 0.3692 | 0.4048 | 0.912 | 0.3705 |
| TOC | 0.8693 | 0.5733 | 1.516 | 0.1419 |

## Approximate significance of smooth terms:

<table>
<thead>
<tr>
<th>edf</th>
<th>Ref.df</th>
<th>F</th>
<th>p-value</th>
</tr>
</thead>
<tbody>
<tr>
<td>year_day</td>
<td>5</td>
<td>5</td>
<td>2.009</td>
</tr>
</tbody>
</table>

## GCV = 8.8576 Scale est. = 5.1024 n = 33

### 2.2.2 Imputation of COD$_s$ of Influent and Effluent Samples

Measurements from Boog et al. (2019) have shown that for the influent, COD$_s$/DOC was similar to COD/TOC (3–4) and that COD$_t$/COD$_s$ was approximately 2. Therefore, influent COD$_s$ was estimated by combining the mean of DOC/TOC and by 0.5 of the COD; each weighted 50% (Equation XXX).

$$\text{COD}_s = 0.5 \times \text{mean} \left( \frac{\text{COD}_t}{\text{TOC}} \right) \text{DOC} + 0.5 \times \text{mean} \left( \frac{\text{COD}_s}{\text{COD}} \right) \text{COD}$$

COD$_s$ will be imputed by using mean ratios COD/COD$_s$ and rolling means of TOC/DOC COD$_s$/DOC measured during Feb-Apr2018.

### 2.2.3 Imputation of COD$_s$ and COD$_t$ for Pore Water Samples

Following ratios of COD$_t$/TOC and COD$_s$/DOC were derived based on measurements of pore water samples for COD$_t$, COD$_s$, TOC, and DOC by Boog et al. (2019).

- COD$_t$/TOC of 3.0
- COD$_s$/DOC of 3.5

These ratios were used to impute COD$_t$ and COD$_s$ of the pore water samples of the aeration interruption experiments. Note that COD$_t$ was not imputed for corresponding samples of the aeration interruption experiment in July to August 2015 as TOC was not measured.
Figure 6: COD, CODₘ, TOC, DOC concentrations in mg/L as well as ratios of COD to TOC (COD_TOC) and ratio of CODₘ to DOC (CODₘ_DOC) of measured pore water samples of system HA from Boog et al. (2019). Black dots represent individual values, red dots averages.

2.3 Imputation of BCOD Concentration of the Influent

BCOD data was estimated according to Roeleveld and Loosdrecht (2002). At first, the total amount of CBOD (CBODₜot, also termed as ultimate BOD) is computed from CBOD₅ measurements (Equation (1)). Remember, the C in CBOD just explicitly mentions that a nitrification inhibitor was added during the measurement (this is usually implicit for BOD).

\[
CBOD_{tot}(t) = \frac{1}{1 - e^{-k_{CBOD_{10}}}} \times CBOD_5(t)
\]

The rate constant \(k_{CBOD_{10}}\) was determined from CBOD₁₀ curves by Boog et al. (2019) to \(k_{CBOD_{10}} = 2.75 \times 10^{-4}\) 1/d, CBOD₅ measurements of the routine sampling were used.

At second, \(CBOD_{tot}(t)\) was converted into BCOD by dividing through a conversion factor \(f_{BOD}\) (Equation (2)). This is done due compensate for CBOD consumption by bacteria during the measurement itself, as it takes several days (\(f_{BOD} = 0.15\) Roeleveld and Loosdrecht (2002)).

\[
BCOD(t) = \frac{1}{1 - f_{BOD}} \times CBOD_{tot}(t)
\]

If no CBOD₅ measurements were available, BCOD was determined as:
2.4 Simulations

2.4.1 Influent and Effluent Data for Model Calibration and Validation on Aeration Interruption Experiments

Figure 7: Measured and simulated effluent concentrations of *Calibration* and *Validation* scenario of the aeration interruption experiment.
Figure 8: Length profile of measured and simulated NH\textsubscript{4}–N and NO\textsubscript{x}–N concentrations during the 42 days steady–state phase (baseline) of the Calibration scenario. Grey areas indicate median absolute distance of simulations.
Figure 9: Length profile of measured and simulated NH$_4$–N and NO$_x$–N concentrations at 3–6 days after aeration was switched off in the Calibration scenario. Grey areas indicate median absolute distance of simulations.
Figure 10: Length profile of measured and simulated COD concentrations during the 42 days steady–state phase (baseline) of the Calibration scenario. Grey areas indicate median absolute distance of simulations.
Figure 11: Length profile of measured and simulated \( \text{COD}_s \) concentrations at 3–6 days after aeration was switched off in the *Calibration* scenario. Grey areas indicate median absolute distance of simulations.
2.4.2 Additional Figures of Validation on Data of Boog et al. (2019)

![Graph showing measured and simulated effluent concentrations](image)

Figure 12: Measured and simulated effluent concentrations of the scenario *Calibration* of Boog et al. (2019).
Figure 13: Measured and simulated porewater concentrations of the scenario *Calibration* of Boog et al. (2019).
Figure 14: Measured and simulated effluent concentrations of the scenario Cross–Validation of Boog et al. (2019).
Figure 15: Measured and simulated porewater concentrations of the scenario Cross–Validation of Boog et al. (2019).

References

